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The double-exponential transformation in numerical analysis ☆

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Abstract

The double-exponential transformation was first proposed by Takahasi and Mori in 1974 for the efficient evaluation of integrals of an analytic function with end-point singularity. Afterwards, this transformation was improved for the evaluation of oscillatory functions like Fourier integrals. Recently, it turned out that the double-exponential transformation is useful not only for numerical integration but also for various kinds of Sinc numerical methods. The purpose of the present paper is to review the double-exponential transformation in numerical integration and in a variety of Sinc numerical methods.

MSC: 65D30; 65D32

Keywords: Numerical integration; Quadrature formula; Double-exponential transformation; Sinc method; Fourier-type integral

1. Numerical integration and the double-exponential transformation

The double-exponential transformation was first proposed by Takahasi and Mori in 1974 in order to compute the integrals with end-point singularity such as

$$I = \int_{-1}^{1} \frac{\mathrm{d}x}{(2-x)(1-x)^{1/4}(1+x)^{3/4}} \tag{1.1}$$

with high efficiency [7,10,11,30].

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The double-exponential formula for numerical integration based on this transformation can be derived in the following way. Let the integral under consideration be

$$I = \int_a^b f(x)\,\mathrm{d}x. \tag{1.2}$$

The interval (a, b) of integration may be finite, half-infinite $(0, \infty)$ or infinite $(-\infty, \infty)$. The integrand $f(x)$ must be analytic on the interval (a, b) but may have a singularity at the end point $x = a$ or b or both.

Now, we apply a variable transformation

$$x = \phi(t), \quad a = \phi(-\infty), \quad b = \phi(\infty), \tag{1.3}$$

where $\phi(t)$ is analytic on $(-\infty, \infty)$, and have

$$I = \int_{-\infty}^{\infty} f(\phi(t))\phi'(t)\,\mathrm{d}t. \tag{1.4}$$

A crucial point is that we should employ a function $\phi(t)$ such that after the transformation the decay of the integrand be double exponential, i.e.,

$$|f(\phi(t))\phi'(t)| \approx \exp(-c\exp|t|), \quad |t| \to \infty. \tag{1.5}$$

On the other hand, it is known that, for an integral like (1.4) of an analytic function over $(-\infty, \infty)$, the trapezoidal formula with an equal mesh size gives an optimal formula [5,28]. Accordingly, we apply the trapezoidal formula with an equal mesh size h to (1.4), which gives

$$I_h = h \sum_{k=-\infty}^{\infty} f(\phi(kh))\phi'(kh). \tag{1.6}$$

In actual computation of (1.6) we truncate the infinite summation at $k = -N_-$ and $k = N_+$ and obtain

$$I_h^{(N)} = h \sum_{k=-N_-}^{N_+} f(\phi(kh))\phi'(kh), \quad N = N_+ + N_- + 1, \tag{1.7}$$

where N is the number of function evaluations. Since the integrand after the transformation decays double exponentially like (1.5), we call the formula obtained in this way the double-exponential formula, abbreviated as the DE formula.

For the integral over $(-1, 1)$

$$I = \int_{-1}^{1} f(x)\,\mathrm{d}x \tag{1.8}$$

the transformation

$$x = \phi(t) = \tanh\left(\frac{\pi}{2}\sinh t\right) \tag{1.9}$$

will give a double-exponential formula

$$I_h^{(N)} = h \sum_{k=-N_-}^{N_+} f\left(\tanh\left(\frac{\pi}{2}\sinh kh\right)\right) \frac{\pi/2\cosh kh}{\cosh^2(\pi/2\sinh kh)}. \tag{1.10}$$

The double-exponential formula is designed so that it gives the most accurate result by the minimum number of function evaluations. In this sense, we call it an optimal formula [30]. For example, in

Table 1
Comparison of the efficiency of DEFINT and DQAGS. The absolute error tolerance is 10^{-8}. N is the number of function evaluations and abs.error is the actual absolute error of the result

	DEFINT		DQAGS	
Integral	N	abs.error	N	abs.error
I_1	25	$2.0 \cdot 10^{-11}$	315	$6.7 \cdot 10^{-16}$
I_2	387	$4.8 \cdot 10^{-14}$	189	$3.1 \cdot 10^{-15}$
I_3	387	$1.0 \cdot 10^{-13}$	567	$1.1 \cdot 10^{-13}$
I_4	259	$4.8 \cdot 10^{-12}$	651	$1.4 \cdot 10^{-17}$

case of (1.1), it gives an approximate value which is correct up to 16 significant digits by only about $N = 50$ function evaluations.

The merits of the double-exponential formula are as follows.

First, if we write the error of (1.6) in terms of the mesh size h of the trapezoidal formula, we have [30]

$$|\Delta I_h| = |I - I_h| \approx \exp\left(-\frac{c_1}{h}\right). \tag{1.11}$$

From this we see that the error converges to 0 very quickly as the mesh size h becomes small. On the other hand, if we write the error in terms of the number N of function evaluations, we have [30]

$$|\Delta I_h^{(N)}| = |I - I_h^{(N)}| \backsimeq \exp\left(-c_2 \frac{N}{\log N}\right). \tag{1.12}$$

A single-exponential transformation

$$x = \tanh t \tag{1.13}$$

for the integral over $(-1, 1)$ will give [30]

$$|\Delta I_h^{(N)}| \approx \exp(-c_3\sqrt{N}). \tag{1.14}$$

We can see that as N becomes large, (1.12) converges to 0 much more quickly than (1.14).

Second, if the integrand has a singularity at the end point like (1.1), it will be mapped onto infinity. On the other hand, the integrand after the transformation decays double exponentially toward infinity, and hence we can truncate the infinite summation at a moderate value of k in (1.6). In addition, we can evaluate integrals with different orders of singularity using the same formula (1.7). In that sense, we can say that the double-exponential formula is robust with regard to singularities.

Third, since the base formula is the trapezoidal formula with an equal mesh size, we can make use of the result of the previous step with the mesh size h when we improve the value by halving the mesh size to $h/2$. Therefore, the present formula is suitable for constructing an automatic integrator. In addition, the points $\phi(kh)$ and the weights $h\phi'(kh)$ can easily be computed as seen in (1.10).

In Table 1 we show numerical examples to compare the efficiency of an automatic integrator DEFINT in [8] based on the DE transformation (1.9) and DQAGS in QUADPACK [24] for the following four integrals:

$$I_1 = \int_0^1 x^{-1/4} \log(1/x)\,\mathrm{d}x, \qquad I_2 = \int_0^1 \frac{1}{16(x - \pi/4)^2 + 1/16}\,\mathrm{d}x,$$

$$I_3 = \int_0^{\pi} \cos(64 \sin x)\,\mathrm{d}x, \qquad I_4 = \int_0^1 \exp(20(x-1))\sin(256x)\,\mathrm{d}x.$$

From Table 1 we see that DEFINT is more efficient than DQAGS for I_1, I_3 and I_4, but that it is less efficient for I_2 because its integrand has a sharp peak at $x = \pi/4$ and DEFINT regards it as almost not analytic at this point.

The double-exponential transformation can be applied not only to an integral with end-point singularity over a finite interval, but also to other kinds of integrals such as an integral over a half-infinite interval [9]. Some useful transformations for typical types of integrals are listed below:

$$I = \int_{-1}^{1} f(x)\,\mathrm{d}x \Rightarrow x = \tanh\left(\frac{\pi}{2}\sinh t\right), \tag{1.15}$$

$$I = \int_{0}^{\infty} f(x)\,\mathrm{d}x \Rightarrow x = \exp\left(\frac{\pi}{2}\sinh t\right), \tag{1.16}$$

$$I = \int_{0}^{\infty} f_1(x)\exp(-x)\,\mathrm{d}x \Rightarrow x = \exp(t - \exp(-t)), \tag{1.17}$$

$$I = \int_{-\infty}^{\infty} f(x)\,\mathrm{d}x \Rightarrow x = \sinh\left(\frac{\pi}{2}\sinh t\right). \tag{1.18}$$

Before the double-exponential formula was proposed, a formula by Iri et al. [2], abbreviated as IMT formula, based on the transformation which maps $(-1, 1)$ onto itself had been known. This transformation gave a significant hint for the discovery of the double-exponential formula [29]. However, the error of the IMT formula behaves as $\exp(-c\sqrt{N})$, which is equivalent to the behavior of a formula based on the single-exponential transformation like (1.13). Also, there have been some attempts to improve the efficiency of the IMT formula [6,12].

In a mathematically more rigorous manner, the optimality of the double-exponential formula is established by Sugihara [26]. His approach is functional analytic. The basis of this approach is due to Stenger, which is described in full detail in his book [25]. Stenger there considers the integral $\int_{-\infty}^{\infty} g(w)\,\mathrm{d}w$ as the complex integral along the real axis in the w-plane and supposes that the integrand $g(w)$ is analytic and bounded in the strip region $|\mathrm{Im}\, w| < d$ of the w-plane. Under some additional conditions, he proves that the trapezoidal rule with an equal mesh size is optimal for the integral of a function which decays single exponentially as $w \to \pm\infty$ along the real axis. He also shows that the error behaves like (1.14). Sugihara proceeds analogously. He supposes that the integrand $g(w)$ be analytic and bounded in the strip region $|\mathrm{Im}\, w| < d$ of the w-plane, and proves the optimality of the trapezoidal rule with an equal mesh size for the integral of a function enjoying the double-exponential decay, together with an error estimate like (1.12). This result shows that the double-exponential transformation provides a more efficient quadrature formula than the single exponential one. Sugihara further shows that, except the identically vanishing function, there exists no function that is analytic and bounded in the strip region $|\mathrm{Im}\, w| < d$ and that decays more rapidly than $\exp(-\exp(\pi/2d|w|))$ as $w \to \pm\infty$. Thus, he concludes that the double-exponential formula is optimal.

2. Evaluation of Fourier-type integrals

Although the double-exponential transformation is useful for various kinds of integrals, it does not work well for Fourier-type integrals of a slowly decaying oscillatory function like

$$I_s = \int_0^\infty f_1(x)\sin\omega x\,\mathrm{d}x,$$
$$I_c = \int_0^\infty f_1(x)\cos\omega x\,\mathrm{d}x. \tag{2.1}$$

In 1991 Ooura and Mori proposed a variable transformation suitable for such kinds of integrals [21]. Choose a function $\phi(t)$ satisfying

$$\phi(-\infty) = 0, \quad \phi(+\infty) = \infty, \tag{2.2}$$

$$\phi'(t) \to 0 \quad \text{double exponentially as } t \to -\infty, \tag{2.3}$$

$$\phi(t) \to t \quad \text{double exponentially as } t \to +\infty, \tag{2.4}$$

and transform I_s and I_c using

$$\begin{cases} I_s : x = M\phi(t)/\omega \\ I_c : x = M\phi\left(t - \dfrac{\pi}{2M}\right)\Big/\omega \end{cases} \qquad (M = \text{const.}). \tag{2.5}$$

Then we have a new kind of the double-exponential formula useful for the integrals such as (2.1). M is a constant which will be determined as shown later. This transformation is chosen in such a way that as x becomes large in the positive direction the points of the formula approach double exponentially the zeros of $\sin\omega x$ or $\cos\omega x$, so that we do not have to evaluate the integrand for large value of x.

Ooura and Mori first proposed a transformation

$$\phi(t) = \frac{t}{1 - \exp(-k\sinh t)}, \tag{2.6}$$

which satisfies the condition mentioned above [21]. Afterwards, Ooura proposed

$$\phi(t) = \frac{t}{1 - \exp(-2t - \alpha(1 - \mathrm{e}^{-t}) - \beta(\mathrm{e}^{t} - 1))} \tag{2.7}$$

$$\beta = \tfrac{1}{4}, \quad \alpha = \beta/\sqrt{1 + M\log(1 + M)/(4\pi)} \tag{2.8}$$

as a more efficient transformation [18,20,23].

Table 2
Comparison of the efficiency of a DE integrator and DQAWF. While 10^{-8} is given as the absolute error tolerance for DQAWF, it is given as the relative error tolerance for the DE integrator. N is the number of function evaluations, and rel.error and abs.error are the actual relative and absolute errors of the result

	DE integrator			DQAWF	
Integral	N	rel.error	abs.error	N	abs.error
I_5	72	$1.0 \cdot 10^{-14}$	$1.6 \cdot 10^{-14}$	430	$1.8 \cdot 10^{-11}$
I_6	308	$3.6 \cdot 10^{-11}$	$2.0 \cdot 10^{-11}$	445	$2.7 \cdot 10^{-11}$
I_7	70	$1.2 \cdot 10^{-10}$	$6.9 \cdot 10^{-11}$	570	$6.8 \cdot 10^{-12}$
I_8	68	$1.0 \cdot 10^{-14}$	$1.3 \cdot 10^{-14}$	615	$1.4 \cdot 10^{-11}$

If we substitute $\phi(t)$ into x of I_s in (2.1) we have

$$I_s = M \int_{-\infty}^{\infty} f_1(M\phi(t)/\omega) \sin(M\phi(t))\phi'(t)/\omega \, \mathrm{d}t. \tag{2.9}$$

Then, we apply the trapezoidal formula with an equal mesh size h and have

$$I_{s,h}^{(N)} = Mh \sum_{k=-N_-}^{N_+} f_1(M\phi(kh)/\omega) \sin(M\phi(kh))\phi'(kh)/\omega. \tag{2.10}$$

The situation is similar in the case of I_c. Here we choose M and h in such a way that

$$Mh = \pi. \tag{2.11}$$

Then for I_s as well as I_c

$$\sin(M\phi(kh)) \sim \sin Mkh = \sin \pi k = 0,$$

$$\cos\left(M\phi\left(kh - \frac{\pi}{2M}\right)\right) \sim \cos\left(Mkh - \frac{\pi}{2}\right) = \cos\left(\pi k - \frac{\pi}{2}\right) = 0 \tag{2.12}$$

hold, and we see that as k becomes large the points approach the zeros of $\sin \omega x$ or $\cos \omega x$ double exponentially.

The formula gives a good result even when it is applied to an integral

$$I = \int_0^{\infty} \log x \sin x \, \mathrm{d}x = -\gamma \tag{2.13}$$

whose integrand has a divergent function $\log x$ [22]. Although this integral should be defined as

$$\lim_{\varepsilon \to 0} \int_0^{\infty} \exp(-\varepsilon x) \log x \sin x \, \mathrm{d}x = -\gamma, \tag{2.14}$$

we will get an approximate value of $-\gamma$ that is correct up to 10 significant digits with only 70 function evaluations of $f_1(x) = \log x$ in the formula (2.10).

In Table 2, we show numerical examples of Fourier-type integrals to compare the efficiency of a DE automatic integrator based on the DE transformation (2.7) and (2.8), and DQAWF in QUADPACK [24] for the following four integrals:

$$I_5 = \int_0^{\infty} \frac{\sin x}{x} \, \mathrm{d}x, \qquad I_6 = \int_0^{\infty} \frac{\cos x}{(x-2)^2 + 1} \, \mathrm{d}x,$$

$$I_7 = \int_0^\infty \log x \sin x \,\mathrm{d}x, \qquad I_8 = \int_0^\infty \frac{\cos x}{\sqrt{x}} \,\mathrm{d}x.$$

3. Application of the double-exponential transformation to other types of integrals

The double-exponential transformation can be used to evaluate other kinds of integrals.

Ogata et al. proposed a method to evaluate the Cauchy principal value integral

$$I = \mathrm{p.v.} \int_{-1}^{1} \frac{f(x)}{x-\lambda} \,\mathrm{d}x \tag{3.1}$$

and the Hadamard finite-part integral

$$I = \mathrm{f.p.} \int_{-1}^{1} \frac{f(x)}{(x-\lambda)^n} \,\mathrm{d}x \tag{3.2}$$

by means of the double-exponential transformation [16].

Ogata and Sugihara also proposed a quadrature formula for oscillatory integrals involving Bessel functions such as

$$I = \int_0^\infty \frac{x}{x^2+1} J_0(x) \,\mathrm{d}x, \tag{3.3}$$

employing the same idea as mentioned in Section 2 [13–15]. It is noted here that, while developing the quadrature formula, they achieved an extremely high-precision quadrature formula of interpolatory type for antisymmetric integrals, i.e.,

$$I = \int_{-\infty}^{\infty} (\operatorname{sign} x) f(x) \,\mathrm{d}x = \left(\int_0^\infty - \int_{-\infty}^0 \right) f(x) \,\mathrm{d}x. \tag{3.4}$$

The abscissae of the quadrature are zeros of Bessel functions.

Ooura devised a transformation which can be regarded as a continuous version of the Euler transformation. By this transformation, together with the double exponential one, we can evaluate integrals of a slowly decaying oscillatory function like

$$I = \int_0^\infty J_0\left(\sqrt{2x+x^2}\right) \mathrm{d}x \tag{3.5}$$

whose distribution of the zeros is not equidistant [17,20].

Also Ooura combined his continuous Euler transformation with FFT to give a method for efficient evaluation of a Fourier transform [19,20] like

$$I = \frac{1}{2\pi} \int_{-\infty}^{\infty} \log(1+x^2)\, \mathrm{e}^{-\mathrm{i}\omega x} \,\mathrm{d}x. \tag{3.6}$$

4. Sinc numerical methods and the double-exponential transformation

Recently, it turned out that the double-exponential transformation is useful not only for numerical integration but also for a variety of so-called Sinc numerical methods.

The Sinc numerical methods are based on an approximation over the doubly infinite interval $(-\infty,\infty)$, which is written as

$$f(x) \approx \sum_{k=-n}^{n} f(kh)S(k,h)(x), \tag{4.1}$$

where the basis functions $S(k,h)(x)$ are the Sinc functions defined by

$$S(k,h)(x) = \frac{\sin \pi/h(x-kh)}{\pi/h(x-kh)}, \quad k = 0, \pm 1, \pm 2, \ldots, \tag{4.2}$$

with a positive constant h. The approximation (4.1) is called the Sinc approximation.

The Sinc approximation and numerical integration are closely related through an identity

$$\int_{-\infty}^{\infty} \left(\sum_{k=-n}^{n} f(kh)S(k,h)(x) - f(x) \right) \mathrm{d}x = h \sum_{k=-n}^{n} f(kh) - \int_{-\infty}^{\infty} f(x)\, \mathrm{d}x \tag{4.3}$$

between the approximation error of the Sinc approximation and the one of integration by the trapezoidal rule. This identity implies that the class of the functions for which the Sinc approximation gives highly accurate approximations is almost identical to the class of functions for which the trapezoidal rule gives highly accurate results. This fact suggests that the applicability of the transformation technique developed in the area of numerical integration of the Sinc approximation, even further to the Sinc numerical methods. In fact, in [25], the standard treatise of the Sinc numerical methods, the single-exponential transformation is assumed to be employed. But why not the double-exponential transformation? Recently, Sugihara and his colleagues have started to examine the applicability of the double-exponential transformation to a variety of Sinc numerical methods.

In the most fundamental case, i.e., in the Sinc approximation, Sugihara makes a full study of the error, thereby proving that when the double-exponential transformation is employed, the optimal result is obtained just as in numerical integration [27].

Horiuchi and Sugihara combine the double-exponential transformation with the Sinc-Galerkin method for the second-order two-point boundary problem [1]. To be specific, consider

$$\begin{aligned} &\tilde{y}''(x) + \tilde{\mu}(x)\tilde{y}'(x) + \tilde{v}(x)\tilde{y}(x) = \tilde{\sigma}(x), \quad a < x < b, \\ &\tilde{y}(a) = \tilde{y}(b) = 0. \end{aligned} \tag{4.4}$$

Application of the variable transformation

$$x = \phi(t), \quad a = \phi(-\infty), \quad b = \phi(\infty), \tag{4.5}$$

together with the change of notation

$$y(t) = \tilde{y}(\phi(t)), \tag{4.6}$$

transforms the problem to

$$\begin{aligned} &y''(t) + \mu(t)y'(t) + v(t)y(t) = \sigma(t), \quad -\infty < t < \infty, \\ &y(-\infty) = y(\infty) = 0. \end{aligned} \tag{4.7}$$

The Sinc-Galerkin method approximates the solution of the transformed problem (4.7) by a linear combination of the Sinc functions:

$$y_N(t) = \sum_{k=-n}^{n} w_k S(k,h)(t), \quad N = 2n+1. \tag{4.8}$$

It is shown by both theoretical analysis and numerical experiments that the approximation error can be estimated by

$$|y(t) - y_N(t)| \leqslant c' N^{5/2} \exp(-c\sqrt{N}) \tag{4.9}$$

if the true solution $y(t)$ of the transformed problem decays single exponentially like

$$|y(t)| \leqslant \alpha \exp(-\beta|t|). \tag{4.10}$$

It is also shown that the approximation error can be estimated by

$$|y(t) - y_N(t)| \leqslant c' N^2 \exp\left(-\frac{cN}{\log N}\right) \tag{4.11}$$

if the true solution $y(t)$ of the transformed problem decays double exponentially like

$$|y(t)| \leqslant \alpha \exp(-\beta \exp(\gamma|t|)). \tag{4.12}$$

Evidently, the error estimates (4.9) and (4.11) show the superiority of the double-exponential transformation. By the analogy with the case of the Sinc approximation we believe that the error estimate (4.11) should be best possible, i.e., the double-exponential transformation should be optimal, though it has not been proved yet.

Koshihara and Sugihara study the performance of the double-exponential transformation when used in the Sinc-Collocation method for the Sturm–Liouville eigenvalue problems. It is shown that the error behaves like (4.11) [3].

Matsuo applies the double-exponential transformation to the Sinc-pseudospectral method for the nonlinear Schrödinger equation and reports that a highly accurate numerical solution is obtained [4].

As seen above, the double-exponential transformation has proved to be a useful tool in numerical analysis in a number of areas. We believe that the double-exponential transformation should prove to be effective even in wider areas of numerical analysis.

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